EFFICIENT NON-FOURIER IMPLEMENTATION OF LANDAU-FLUID OPERATORS IN THE BOUT++ CODE

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Motivation and Introduction

- Effective phase-mixing damping rate in Landau-fluid closure

$$\gamma \propto -\left|k_{\shortparallel}\right| v_{\mathrm{th}}$$

- Specific example, with collisions

$$\nabla_{\shortparallel} Q_{\shortparallel}(z) \approx -8 n_0 v_{\mathrm{th}}^2 \int dk_{\shortparallel}\, e^{ik_{\shortparallel} z} \frac{k_{\shortparallel}^2 \tilde{T}_{\shortparallel}}{\sqrt{8\pi}\left|k_{\shortparallel}\right| v_{\mathrm{th}} + (3\pi - 8)\,\nu_s}$$

- Such operators are easy to represent and efficient to calculate in Fourier $(k_{\shortparallel})$ space.
- When large (including background) spatial inhomogeneities are present in the phase-mixing operators, evaluation using Fourier methods becomes inefficient.

- With mesh-based schemes (finite difference, volume, element, etc.), it is straightforward to construct approximations to $(\nabla_{\shortparallel})^n \leftrightarrow (ik_{\shortparallel})^n$, but harder for, e.g., $|k_{\shortparallel}| \times k_{\shortparallel}^n = \mathrm{sgn}\,(k_{\shortparallel}) \times k_{\shortparallel}^{n+1}$.
  - not local in configuration space
- Direct use of the corresponding discretized configuration space kernel by convolution or matrix multiplication is potentially expensive.
  - N_g^2 scaling vs. $N_g \log (N_g)$ of computational expense
- ACCURATE APPROXIMATIONS ARE POSSIBLE THAT CAN BE IMPLEMENTED WITH FOURIER-LIKE SCALING.

Basic idea

- Approximate $1/|k|$ as a sum of suitably scaled Lorentzians

$$\frac{1}{|k|} \approx \sum_{n=0}^{N} \frac{\alpha^n}{k^2 + \alpha^{2n}}$$

- Each individual component of the sum has the correct parity, but asymptotic dependence $1/k^2$ for large k.
- With the above scaling of the height and width, successive terms approximately "fill in" successively higher parts of the $1/|k|$ curve
- The sum provides a quite good fit over some spectral range, which increases with N
- Lorentzians in k space are inverses of Helmholtz operators in real space

Approximate calculation

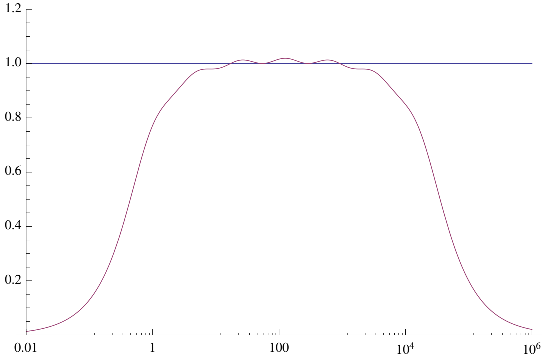
- Discretize the Helmholtz equations
- Solve via a tridiagonal (for 2-point differences) or banded (for higher-order differences) matrix solution
- Direct solvers should work well
  - the matrices are well conditioned
  - parallelizeable along direction of solve
- Sum the results of the matrix solves

Accuracy of the basic approximation

- Look at how close to $\operatorname{sgn}(k) = k/|k|$ is

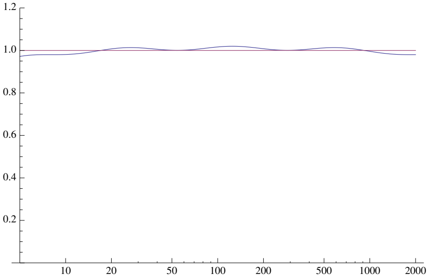
$$\psi(k;\alpha,\beta,N) = \beta k \sum_{n=0}^{N-1} \frac{\alpha^n}{k^2+\alpha^{2n}} \; ?$$

- $\alpha = 5, \beta = 1.04, N = 7$



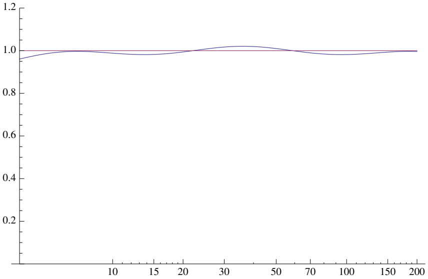
Accuracy of the basic approximation

$\alpha = 5, \beta = 1.04, N = 7$



$k_{\mathrm{min}}/k_{\mathrm{max}} = 400$

$\alpha = 6, \beta = 1.16, N = 5$

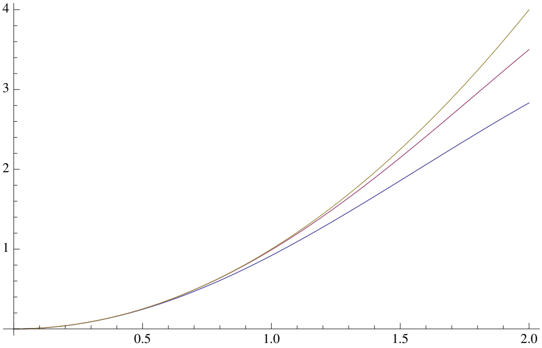


$k_{\mathrm{min}}/k_{\mathrm{max}} = 50$

Finite-grid effects

Compare exact, 3-point and 5-point approximations to k^2

$$
\begin{aligned}
& k^2 \\
K_2^2(k\Delta) &= [2\sin(k\Delta/2)/\Delta]^2 \\
K_4^2(k\Delta) &= \frac{4}{3}[2\sin(k\Delta/2)/\Delta]^2 - \frac{1}{3}[\sin(k\Delta)/\Delta]^2
\end{aligned}
$$



Finite-grid effects

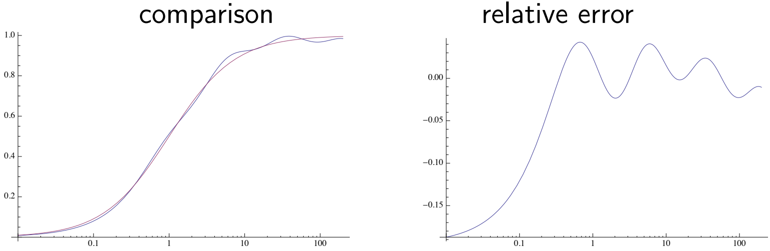
- Finite differences good to some $k_d = \hat{k}_d/\Delta$; $k_d \approx 0.8$ for 3-point; $k_d \approx 1.6$ for 5-point
- Given $\psi\left(\hat{k}\right)$ which fits the desired operator well for $\hat{k}_{min} \lesssim \hat{k} \lesssim \hat{k}_{max}$, scale $\hat{k}$ by factor λ so that $\lambda\hat{k}_{max} = \hat{k}_d/\Delta$, i.e., $\lambda = \hat{k}_d/\left(\hat{k}_{max}\Delta\right)$.
- Then $\psi\left(k/\lambda\right) = \psi\left(k\Delta\hat{k}_{max}/\hat{k}_d\right)$ gives a good fit for $\hat{k}_d\hat{k}_{min}/\hat{k}_{max} \lesssim k\Delta \lesssim \hat{k}_d$, i.e., for all modes in system for $L \lesssim 2\Delta\hat{k}_{max}/\hat{k}_{min}$.

Include collisions

- Can scale operator fit problem to obtaining a fit to $k/\left(|k|+1\right)$
- Can obtain reasonable fit by adjusting coefficient of first Lorentzian

$$\psi\left(k;\alpha,\beta,N\right)=\beta k\left[\frac{\eta}{k^2+1}+\sum_{n=1}^{N}\frac{\alpha^n}{k^2+\alpha^{2n}}\right]$$

- $\alpha=6,\beta=1.15,N=5,\eta=0.5$



Implementation

- Non-Fourier approximation to $1/|k|$ and $-|k|$ operator.

$$
\begin{aligned}
1/|k| &\approx \beta \sum_{n=0}^{N} \frac{\alpha^n}{k^2 + (\alpha^n k_0)^2} \\
-|k| &= -\frac{k^2}{|k|} \approx -\beta \sum_{n=0}^{N} \alpha^n + \beta \sum_{n=0}^{N} \frac{\alpha^{3n} k_0^2}{k^2 + (\alpha^n k_0)^2}
\end{aligned}
$$

- Use 3-point second difference for second derivative

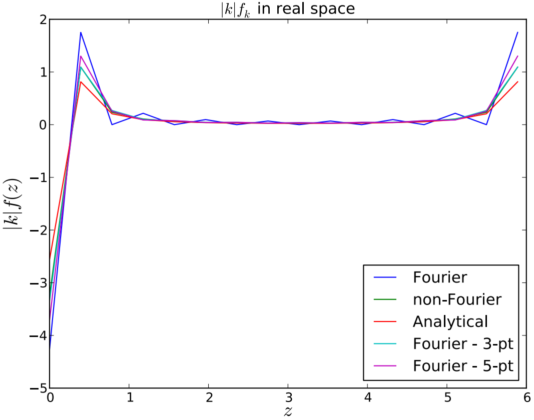
$$
\begin{aligned}
\frac{\partial^2 \psi}{\partial z^2} &\rightarrow \frac{1}{\Delta^2} \left(\psi_{i+1} + \psi_{i-1} - 2\psi_i\right) \\
\therefore\ k^2 &\rightarrow K_2^2(k\Delta) = \left[2\sin(k\Delta/2)/\Delta\right]^2
\end{aligned}
$$

- Periodic domain; "periodic tridiagonal" routine.

Spatial Oscillations (Gibbs Phenomenon) for $-|k|$ Operator

- $\alpha = 5, N = 7, \beta = 1.04.$
- System length$= 2\pi$; 16 grid cells

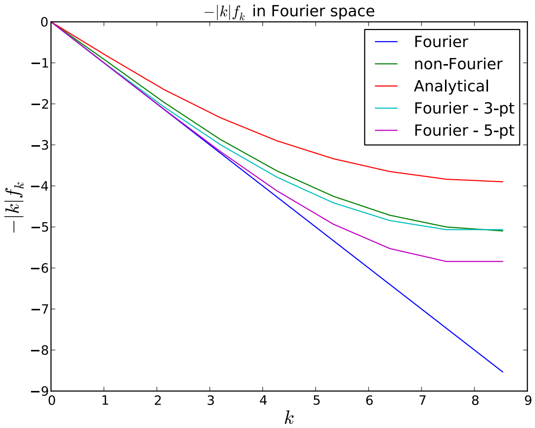
Real Space



Spatial Oscillations (Gibbs Phenomenon) for $-|k|$ Operator

- $\alpha = 5, N = 7,\ \beta = 1.04.$
- System length$= 2\pi$; 16 grid cells

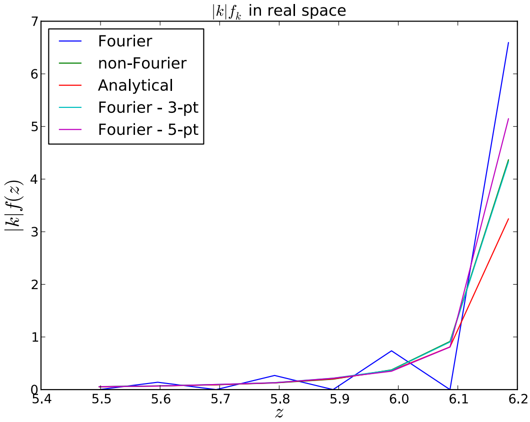
Fourier Space



Spatial Oscillations (Gibbs Phenomenon) for $-|k|$ Operator

- $\alpha = 5, N = 7,\ \beta = 1.04.$
- System length$= 2\pi$; 16 grid cells

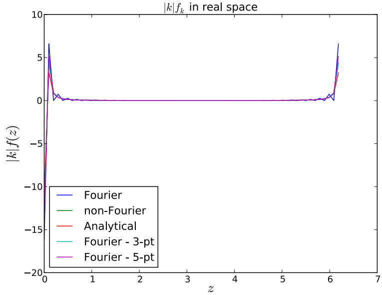
Real Space

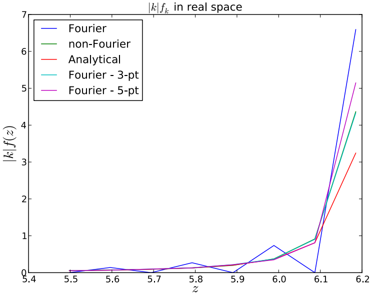


Spatial Oscillations (Gibbs Phenomenon) for $-|k|$ Operator

- $\alpha = 5, N = 7,\ \beta = 1.04.$
- System length$= 2\pi$; 64 grid cells

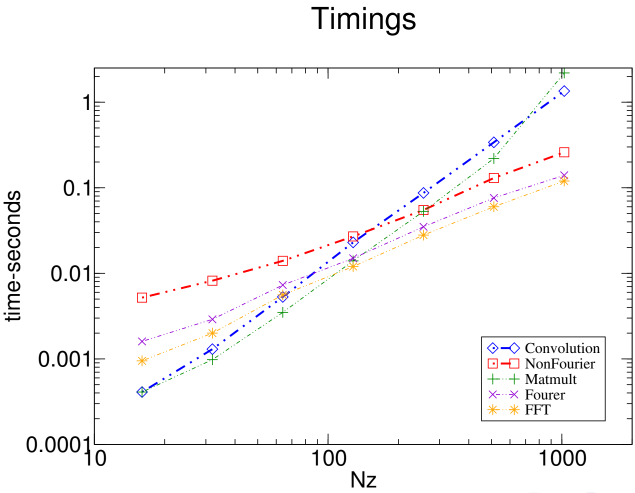
Real Space





Non-Fourier has similar computational scaling to Fourier

- Non-Fourier, with fixed N, scales as N_z, c.f. N_z^2 for direct convolution
- Crossover point is at $N_z \approx 128 \Rightarrow$ advantage for $N_z \gtrsim 200$.



Collocation solution for Laplace inversion ansatz: $\eta_j(k) = b^j/(k^2 + b^{2j})$

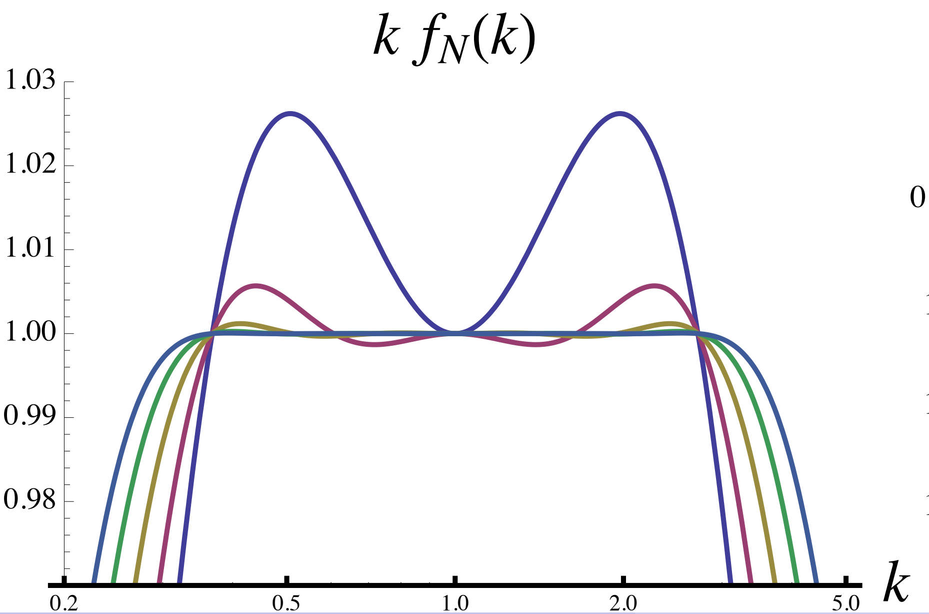
- **Collocation at uniformly spaced points b^i, for $i = -N, \ldots N$ lead to the symmetric linear problem $Ma = 1$ where**

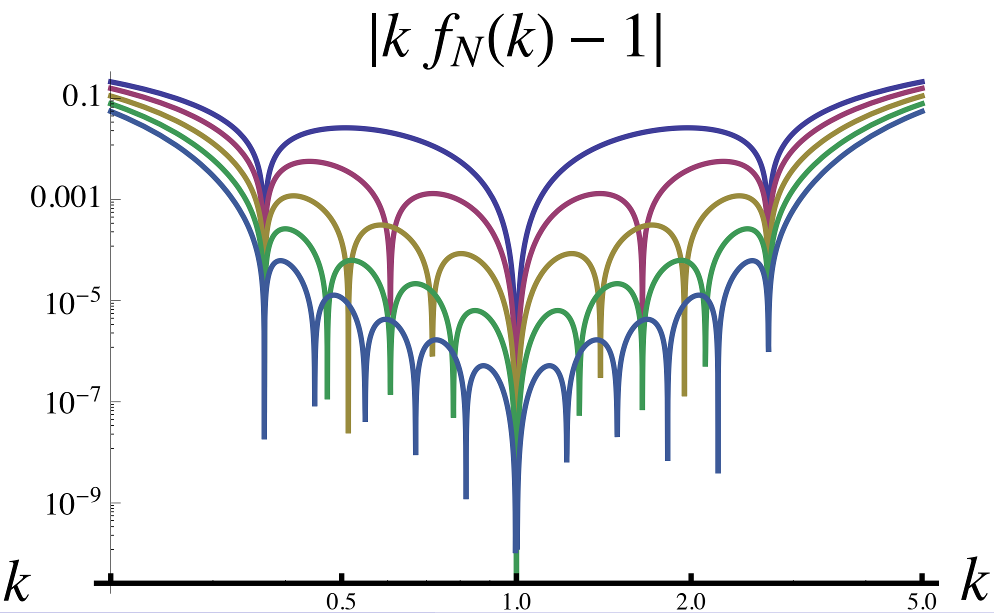
$$M_r^s = b^r b^s/(b^{2r} + b^{2s})$$

- **F4or $b = e$ the solutions are**

N	$2N+1$	$[a^r]$
1	3	[1.84807, 1.68115, 1.84807]
2	5	[1.54322, 0.866876, 1.04278, 0.866876, 1.54322]
3	7	[1.53232, 0.300129, 0.811828, 0.575391, 0.811828, 0.300129, 1.53232]
4	9	[1.70273, -0.263771, 0.885701, 0.293448, 0.656293, . . .]
5	11	[2.01764, -0.999102, 1.27026, -0.110205, 0.727017, 0.127763,. . .]

- **However, error grows at edges of logarithmic interval**





Uniform accuracy can be obtained with Chebyshev collocation points

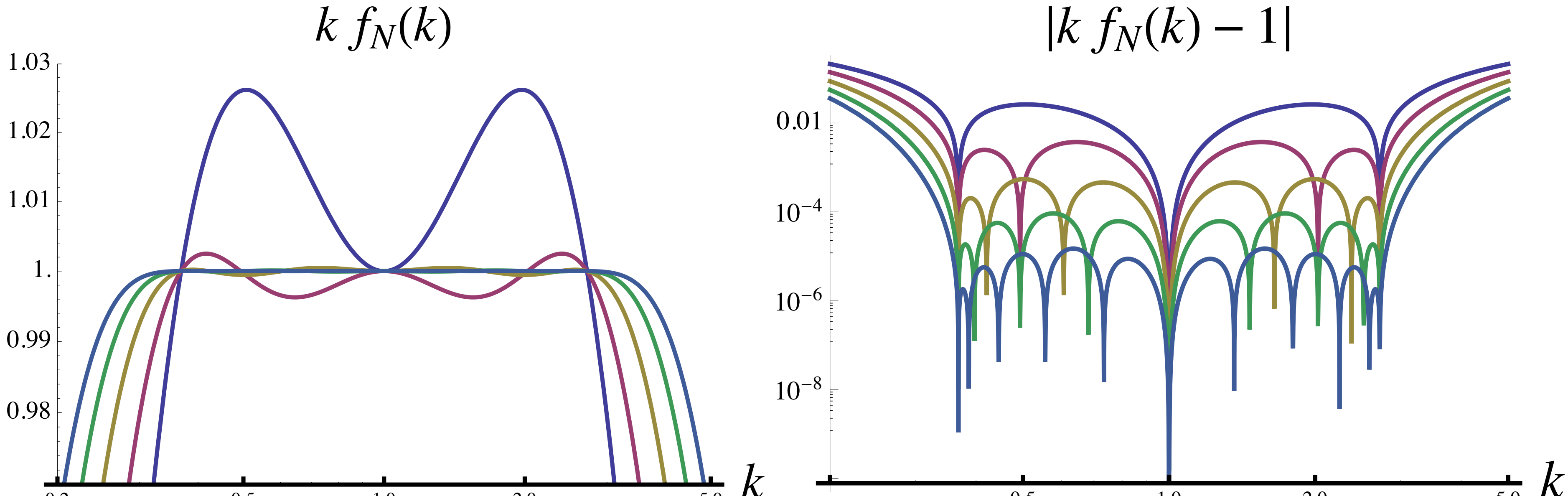
- **Chebyshev polynomial approximation can generate uniform error convergence over the logarithmic interval**
  - For exponential interval b^N, first renormalize by taking the logarithm $\beta = \beta_0 \log b$
  - The Chebyshev collocation points β_s with $2N+1$ polynomials, $s = -N, \ldots N$, are

$$\beta_s = \cos\left((s-N)\pi/2N\right) \qquad \rightarrow \qquad b_s = \exp\left(\beta_0 \cos\left((s-N)\pi/2N\right)\right)$$

- **Chebyshev solution for $\beta_0 = 1$:**

N	$2N+1$	$[a^j]$
1	3	[1.6529, -0.142332, 1.6529]
2	5	[4.06838, -3.65237, 2.52162, -3.65237, 4.06838]
3	7	[16.8245,-22.0064,9.92733,-5.95441, 9.92733, -22.0064, 16.8245]
4	9	[82.5576, -124.155, 62.226, -30.1305, 22.6809, . . .]
5	11	[445.908, -720.514, 409.297, -199.35, 110., -86.8868,. . .]

- **Maximum error is similar, but now more uniform over logarithmic interval**



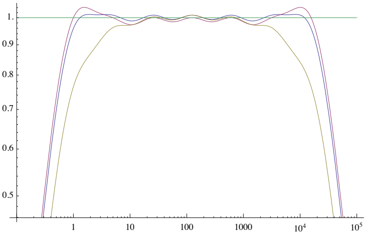
Systematic collocation analysis → improved fits: collisionless

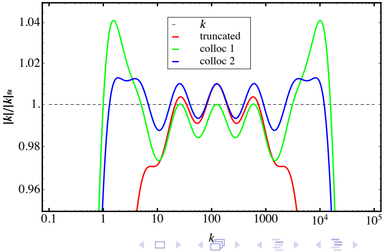
- Collisionless - good (near best) fit is of the form

$$1/|k| \approx \beta \sum_{n=1}^{N} \frac{\zeta_n}{k^2 + (\alpha^{n-1}\kappa_0)^2},$$

- Match exact and approximate forms at collocation points $k = k_n$, $k_n = \alpha^{n-1}\kappa_0$, $n = 2, 3, \ldots, N-1$, $k_0 = \kappa_0/\eta$, $k_N = \eta\alpha^{N-1}\kappa_0$.
- → matrix problem that can be handled e.g., by Mathematica
- Extends spectral range of good fit by ~10-100 for given N, α.

Improved fits vs. original fit





Collisional case introduces a scale length, the mean-free path: λ

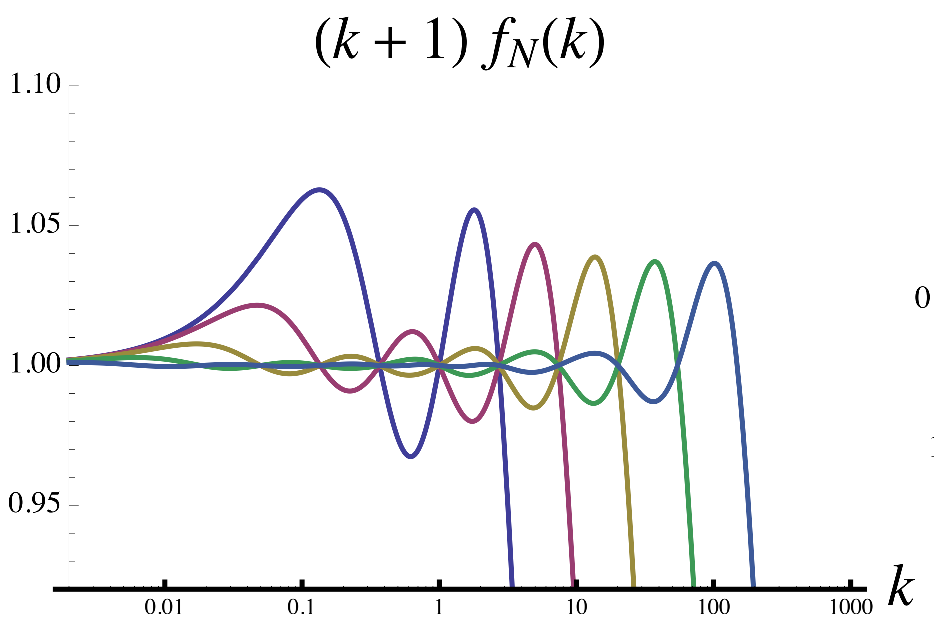
- **Key dimensionless parameter:** $b = k_{max}\lambda$
- **Now, collocation at points** $k\lambda = b^s$ **for** $s = -N, \ldots N$ **generates the equation**

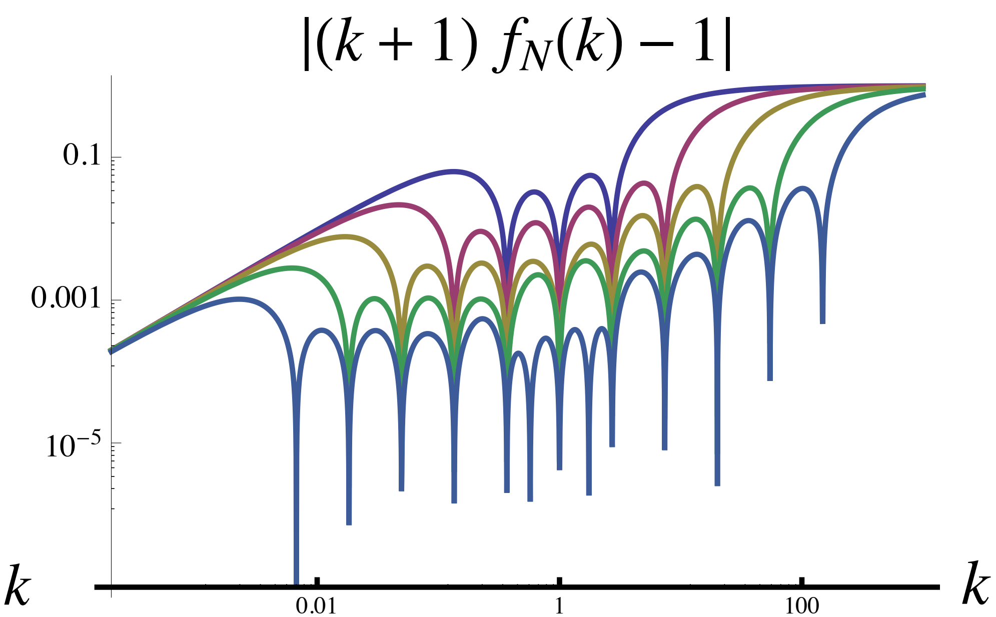
$$M_r^s a^r = b^s/(i + b^s)$$

- **For** $b = e$ **the solutions are**

N	$2N+1$	$[a^j]$
1	3	[0.19703, -0.0711661, 1.45587]
2	5	[0.0280711, 0.0210288, 0.470837, 0.155383, 1.53263]
3	7	[0.00382669, 0.00401212, 0.0966353, 0.261622, 0.714043, 0.219054,1.5438]

- **Again, error grows for the limit** $k\lambda \gg 1$



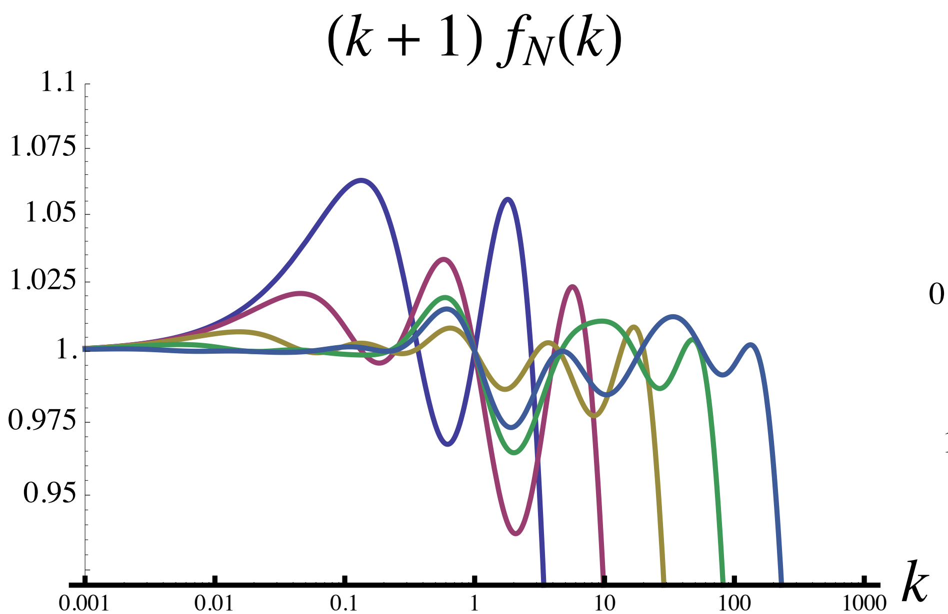


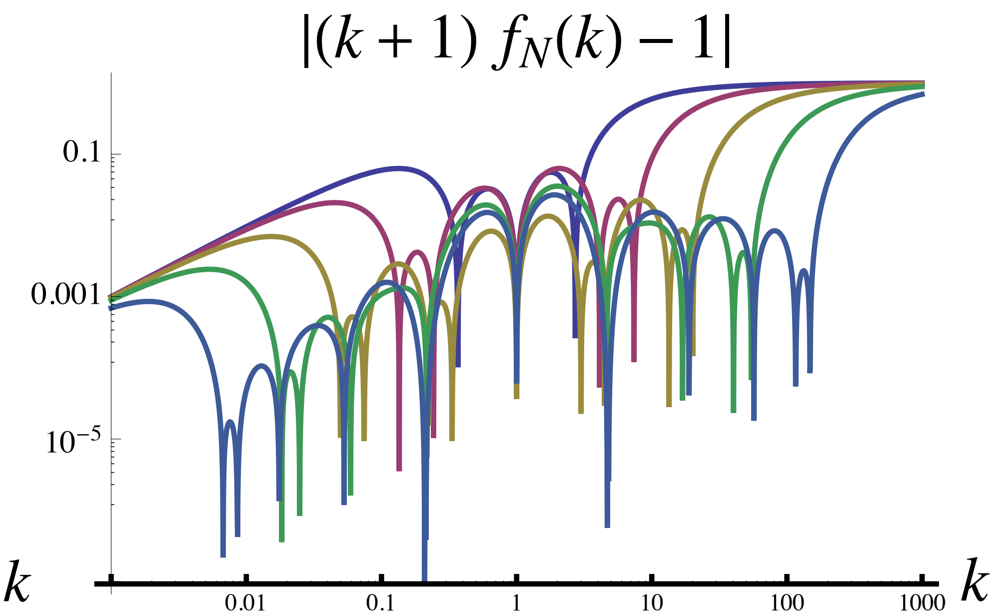
Chebyshev collocation reduces error at large $k \sim k_{max}$

- **Perform collocation at points** $k\lambda = \exp(s\beta_s)$ **where** $\beta_s = \cos((s-N)\pi/2N)$ **and** $s = -N, \ldots N$
- **For** $b = e$ **the solutions are**

N	$2N+1$	$[a^j]$
1	3	[0.19703, -0.0711661, 1.45587]
2	5	[0.0308817, -0.00571965, 0.590679, -0.0967698, 1.68609]
3	7	[0.00571954, -0.00531807, 0.0514562, 0.451945, 1.03353, -0.960316, 2.30743]

- **Still may want to reduce error in middle of domain further ...**





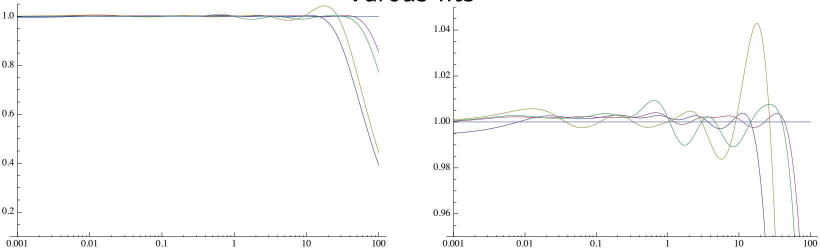
Systematic collocation analysis → improved fits: collisional

- Good (near best) fit is of the form

$$1/\left(1+|k|\right) \approx \beta \sum_{n=-N}^{N} \frac{\zeta_n}{k^2+\alpha^{2n}},$$

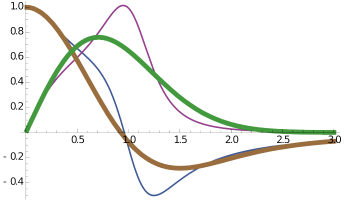
  - collocation points: $k_n = \alpha^n$, $n = -N, \ldots, N-1$, $k_N = \eta\alpha^N$.
- $\alpha = 3,\ 4;\ N = 3,\ 4;\ \eta = 0.5,\ 0.6,\ 1.$

Varous fits



Effect of using sum of Lorentzians on the response functions

- We have implemented a set of Mathematica scripts, which reproduce the HP90 analytic calculations, and also modified them to give the effect of using the sum of Lorentzians for k/|k|.



Using exact k/|k| reproduces the HP90 3-field model.

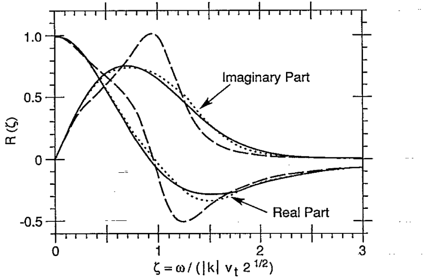
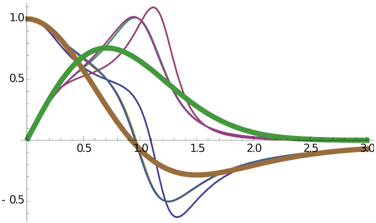


FIG. 1. The real and imaginary parts of the normalized response function $R(\zeta) = -\tilde{n}T_0/n_0 e\tilde{\phi}$ vs the normalized frequency ζ. The solid lines are the exact kinetic result for a Maxwellian, $R(\zeta) = 1 + \zeta Z(\zeta)$. The dashed lines are from the three-moment fluid model with $\Gamma = 3$, $\mu_1 = 0$, and $\chi_1 = 2/\sqrt{\pi}$. The dotted lines are from the four-moment model.

Replacing k/|k| by the sum of Lorentzians approximation yields good fits to the Landau-fluid response functions

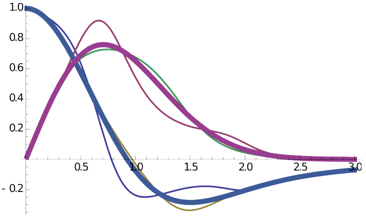
Effect of replacing k/|k| by sum of Lorentzians

3-fluid



$R = R_3\,(k/k_0)$, for $k_0 = 1,\ 10,\ 100.$

4-fluid

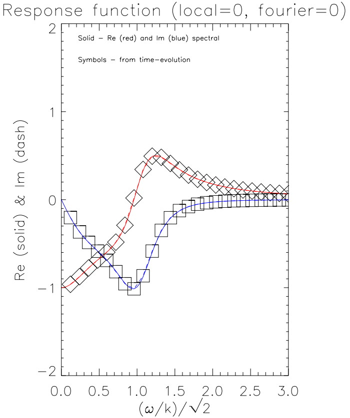


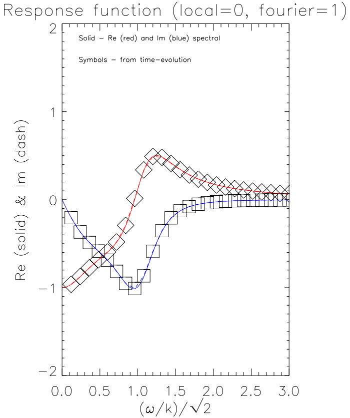
$R = R_4\,(k/k_0)$ for $k_0 = 1,\ 100.$

Replacing k/|k| by the sum of Lorentzians approximation yields good fits to the Landau-fluid response functions

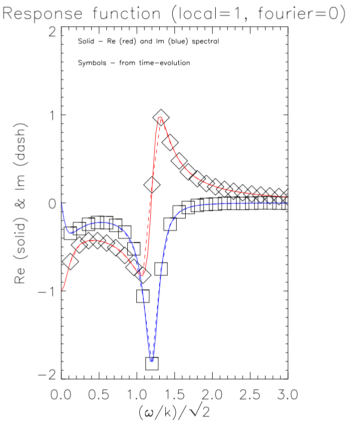
- considered local (q=-chi gradT) and nonlocal (qk=-ik/abs(k) Tk) models for the spectral response function.
- The calculation is done by fourier and non-Fourier methods, for comparison.
- Local non-Fourier means finite-diference, and nonlocal non-Fourier means the Lorentzian method (our main interest).
- Naming convention is: local/nonlocal <=> local=1/0, and similar for Fourier and non-Fourier.

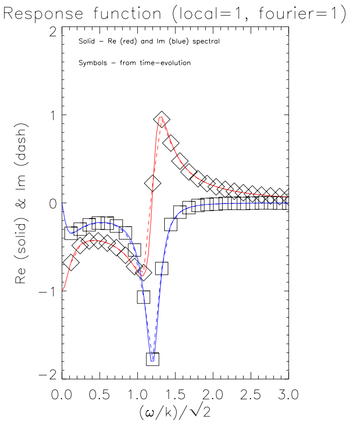
Finite-difference and Fourier implementations of local (diffusive) heat flux in time evolution give response function in agreement with theoretical spectral analysis





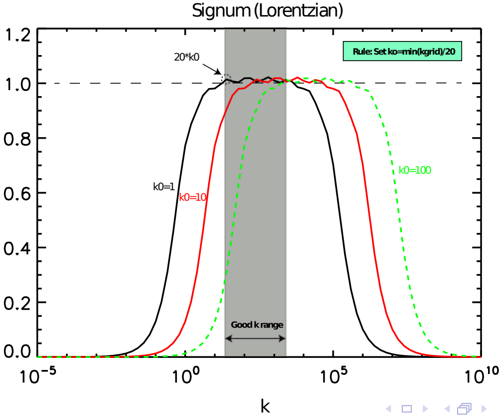
Finite-difference and Fourier implementations of nonlocal heat flux in time evolution give response function in agreement with theoretical spectral analysis





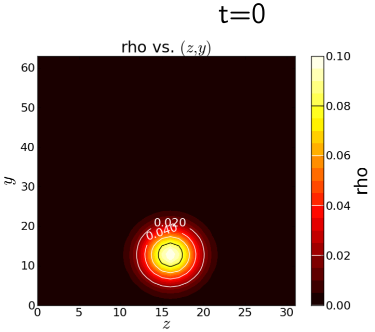
Normalizing wavenumber k_{z0} must be chosen to have region of good fit overlap with resolved modes

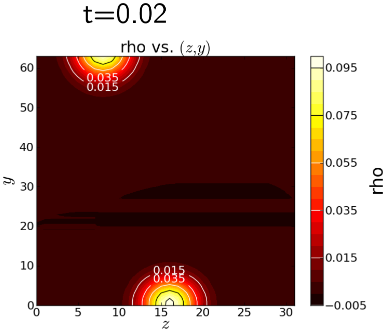
- $k_0 = K_0 * \mathrm{zperiod}$, where K_0 is an $O(1)$ multiplier
- e.g., for parallel case, $\nabla_{||} = (1/h_y)\,\partial_y$, so $k_{||0} = K_{y0}/\sqrt{g_{yy}(y_0)}$.
  - $\sqrt{g_{yy}(y_0)} = h_y(y_0)$ is a measure of the parallel connection length



BOUT++ tests: Parallel advection across parallel boundary

- Gaussian source pulse initialized away from parallel boundary advects across boundary with correct shift

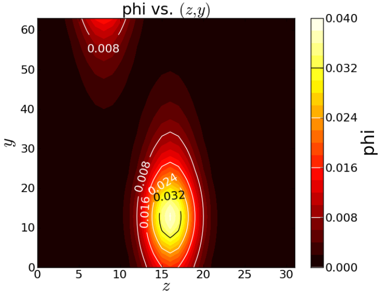




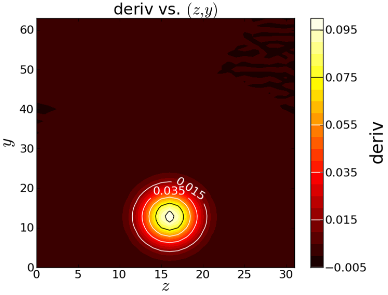
BOUT++ tests: Parallel Laplace Solver

- Parallel (direction) Laplace solver gives sensible solutions with twist-shift boundary condition
- Reconstructed source function is consistent with original source function

Single Helmholtz inversion



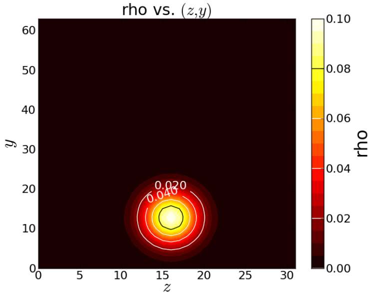
reconstructed source



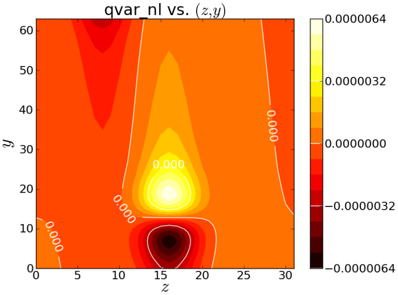
BOUT++ tests: Implementation of non-Fourier sum-of-Lorentzians for parallel Landau-fluid operator

- Non-Fourier LF operator gives sensible solutions with twist-shift boundary condition

Source function



LF flux



Toroidal Landau-fluid ($|\omega_d|$) closure

- Example from Beer '96 - 3+1 equations:

$$
\begin{aligned}
\frac{du_\shortparallel}{dt} &= \text{stuff} - 4i\omega_d u_\shortparallel - 2\left|\omega_d\right| \nu_5 u_\shortparallel \\
\frac{dp_\shortparallel}{dt} &= \text{stuff} - i\omega_d\left(7p_\shortparallel + p_\perp - 4n\right) - 2\left|\omega_d\right|\left(\nu_1 T_\shortparallel + \nu_2 T_\perp\right) \\
\frac{dp_\perp}{dt} &= \text{stuff} - i\omega_d\left(5p_\perp + p_\shortparallel - 3n\right) - 2\left|\omega_d\right|\left(\nu_3 T_\shortparallel + \nu_4 T_\perp\right)
\end{aligned}
$$

Toroidal Landau-fluid ($|\omega_d|$) closure

- Linear forms for $i\omega_d$

$$
\begin{aligned}
i\omega_d\Phi &= i\mathbf{V}_d\cdot\mathbf{k}_\perp\Phi \\
&= \frac{1}{2(T_{\mathrm{norm}}B_0)}\left[\frac{T_{\perp 0}}{B_0}\hat{\mathbf{b}}\times\nabla B_0\cdot\nabla + T_{\parallel 0}\hat{\mathbf{b}}\times\left(\hat{\mathbf{b}}\cdot\nabla\hat{\mathbf{b}}\right)\cdot\nabla\right]\Phi
\end{aligned}
$$

- Need to add correct combination and generalize T_0 to finite amplitude
- To get coefficients for modified version of *invert_laplace*, decompose $\mathbf{V}_d$ and $\nabla\Phi$ into components

$$
\begin{aligned}
\mathbf{V}_d &= V_d^i\mathbf{e}_i \\
\nabla\Phi &= \mathbf{e}^i\partial_i\Phi \\
\mathbf{V}_d\cdot\nabla\Phi &= V_d^i\partial_i\Phi
\end{aligned}
$$

BOUT++ implementation

- Components V_d^1 , V_d^3 easily calculated with existing routines in BOUT++
- Basic Helmholtz equation can be solved using a modified version of existing perpendicular Laplace solver
    - Current equation is of the form

$$\left(c_1 k_\mathrm{z}^2 - c_2 \partial_\psi^2 + c_3\right) \Phi = S$$

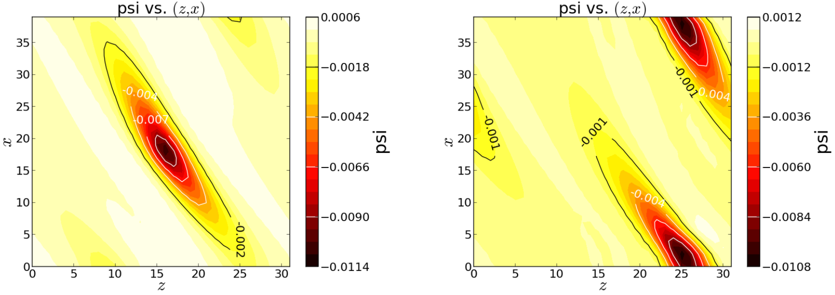
    - Modify to solve

$$\left\{\left[\left(V_d^z\right)^2 k_\mathrm{z}^2 - \left(V_d^\psi\right)^2 \partial_\psi^2 - 2i V_d^\psi V_d^z k_\mathrm{z} \partial_\psi\right] + \alpha^2 \left(V_d^z\right)^2 k_{z0}^2\right\} \Phi = S$$

BOUT++ tests: Perpendicular Laplace solver for $|\omega_d|$ terms

- Perpendicular (direction) Laplace solver gives sensible solutions
- Spreading by Helmholtz inversion is in the same direction as advection

Perp Helmholtz inversion t=0 Perp Helmholtz inversion t=8



(solutions with periodic radial BC's)

Conclusions

- We have developed a new non-Fourier method for the calculation of Landau-fluid operators.
- Useful for situations with large (including background) spatial inhomogeneities.
- Good accuracy (relative error $\lesssim 1\%$ over wide spectral range) is readily achievable.
- Computational cost has value and scaling similar to Fourier method.
- Considerable advantage over direct convolution or matrix multiplication for $N_g \gtrsim 200$.
- Readily applied to toroidal phase-mixing operators ($|\omega_{\mathrm{d}}|$).
- Method is also useful for capturing correct asymptotic form of gyrofluid operators.